IUCLID

DATA SET

Existing Chemicals Linear Alkylbenzene (LAB) Sulfonic Acids (LABSA)

Producer

Company: The LAB Sulfonic Acids Coalition

Creation date: December 5, 2000

Prepared by

Company: THE WEINBERG GROUP INC.

Printing date: March 27, 2003

Revision date:

Date of last update: March 27, 2003

Number of pages: 55

IUCLID

Data Set

Existing Chemical Substance ID: LABSA

Producer Related Part

Company: The Weinberg Group Inc.

Creation date: 05-DEC-2000

Substance Related Part

Company: The Weinberg Group Inc.

Creation date: 05-DEC-2000

Printing date: 27-MAR-2003

Revision date:

Date of last Update: 27-MAR-2003

Number of Pages: 55

Chapter (profile): Chapter: 1, 2, 3, 4, 5, 7

Reliability (profile): Reliability: without reliability, 1, 2, 3, 4

Flags (profile): Flags: without flag, confidential, non confidential, WGK

(DE), TA-Luft (DE), Material Safety Dataset, Risk

Assessment, Directive 67/548/EEC

1.0.1 OECD and Company Information

Name: The LAB Sulfonic Acids Coalition

Remark: The Coalition consists of:

> Colgate - Palmolive Company Akzo Nobel Surface Chemistry LLC

The Dial Corporation

Stepan Company Unilever HPC-USA

21-MAR-2003

1.0.2 Location of Production Site

Not an HPV Challenge endpoint. Remark:

20-FEB-2003

1.0.3 Identity of Recipients

Not an HPV Challenge endpoint. Remark:

20-FEB-2003

1.1 General Substance Information

Substance type: organic Physical status: liquid

Test substance: Benzene sulfonic acid, C10-16-alkyl derivatives (CAS#

68584-22-5)

Benzene sulfonic acid, dodecyl- (CAS# 27176-87-0) Benzene sulfonic acid, tridecyl- (CAS# 25496-01-9)

21-JAN-2002

1.1.1 Spectra

Remark: Not an HPV Challenge endpoint.

20-FEB-2003

1.2 Synonyms

Lauryl benzene sulfonic acid 29-JUN-2001

Alkylbenzene sulfonic acid 29-JUN-2001

- 1/55 -

Benzenesulfonic acid, C10-13-alkyl derivatives (CAS# 85536-14-7) [See assessment report for a discussion of the similarity between this European material and Benzene sulfonic acid, C10-16-alkyl derivatives (CAS# 68584-22-5)] 21-JAN-2002

Dodecyl benzene sulfonic acid 29-JUN-2001

Tridecyl benzene sulfonic acid 29-JUN-2001

1.3 Impurities

CAS-No: **EINECS-No:** EINECS-Name:

Remark: None

02-NOV-2001

1.4 Additives

CAS-No: **EINECS-No: EINECS-Name:**

Remark: None

02-NOV-2001

1.5 Quantity

100 000 - 500 000 tonnes Quantity

05-NOV-2001

1.6.1 Labelling

Labelling:

Not an HPV Challenge endpoint. Remark:

20-FEB-2003

1.6.2 Classification

Classification: Class of danger:

R-Phrases:

Remark: Not an HPV Challenge endpoint.

20-FEB-2003

- 2/55 -

1.7 Use Pattern

Type: Category:

Primarily as an intermediate in the production of LAS. Remark:

02-NOV-2001

1.7.1 Technology Production/Use

Not an HPV Challenge endpoint. Remark:

20-FEB-2003

1.8 Occupational Exposure Limit Values

Type of limit: Limit value:

Remark: No TLV has been established

02-NOV-2001

1.9 Source of Exposure

Memo: No significant exposure. See discussion in accompanying LAB

sulfonic acid assessment plan.

02-NOV-2001

1.10.1 Recommendations/Precautionary Measures

Remark: See LAB sulfonic acid assessment plan.

02-NOV-2001

1.10.2 Emergency Measures

Remark: See LAB sulfonic acid assessment plan.

02-NOV-2001

1.11 Packaging

Bulk transport Memo:

02-NOV-2001

- 3/55 -

1.12 Possib. of Rendering Subst. Harmless

Type of

destruction:

Remark: Not applicable

02-NOV-2001

1.13 Statements Concerning Waste

See LAB sulfonic acid assessment plan. Memo:

02-NOV-2001

1.14.1 Water Pollution

Classified by: Labelled by: Class of danger:

Remark: Not a significant source of water pollution.

02-NOV-2001

1.14.2 Major Accident Hazards

Legislation:

Substance listed:

Remark: None

02-NOV-2001

1.14.3 Air Pollution

Classified by: Labelled by:

Number:

Class of danger:

Remark: Not a significant source of air pollution.

02-NOV-2001

1.15 Additional Remarks

Memo: None

02-NOV-2001

1.16 Last Literature Search

Date of Search: 31-MAY-2001

02-JUL-2001

1.17 Reviews

Memo: None

02-NOV-2001

1.18 Listings e.g. Chemical Inventories

Remark: TSCA inventory (USA)

Domestic Substances List (DSL) - Canada

EINECS (Europe)

21-JAN-2002

- 5/55 -

2.1 Melting Point

= -10 degree C Value:

GLP:

IUCLID cites source as Shell Chemicals U.K. Ltd. Chester Remark:

Test substance: Benzene sulfonic acid, C10-16-alkyl derivatives (68584-22-5)

Reliability: (2) valid with restrictions

21-FEB-2003 (27)

< -10 degree C Value:

GLP:

CONDEA Vista 1995. Source:

Test substance: Alkylbenzene sulfonic acid with the following composition:

Components	CAS Number	Weight%
Nonylbenzenesulfonic Acid	35298-13-6	0.6
n-Decylbenzenesulfonic Acid	140-60-3	18.3
Undecylbenzenesulfonic Acid	50854-94-9	42.1
Dodecylbenzenesulfonic Acid	27176-87-0	30.0
Tridecylbenzenesulfonic Acid	25496-01-9	4.4
Tetradecylbenzenesulfonic Acid	30776-59-1	0.5
Sulfuric Acid	7664-93-9	1.3
Free Oil	None	2.4
Water	7732-18-5	0.4

(4) not assignable Reliability:

Data from Material Safety Data Sheet. No report available for

review.

21-FEB-2003 (4)

= 10 degree C Value:

no data GLP:

Report not available but based on other sources this may Remark:

actually be -10 degrees Celcius.

Source: Verschueren 1996.

Test substance: Benzene sulfonic acid, dodecyl- (27176-87-0)

Reliability: (2) valid with restrictions Peer-reviewed reference book.

21-FEB-2003 (80)

= -10 degree C Value:

no data GLP:

Remark: IUCLID cites source as Hoechst Iberica s.a. Barcelona.

Source: IUCLID 1995.

Test substance: Benzene sulfonic acid, dodecyl- (27176-87-0)

(2) valid with restrictions Reliability:

21-FEB-2003 (28)

- 6/55 -

= 198.5 degree C Value:

Decomposition:

other: Thermal analysis was performed on the Netzsch DSC 204C Method:

and TG209C with N2 atmosphere.

GLP: no

Remark: This measured melting point value is significantly lower than

the EPI Suite estimated values for other LAS materials.

Decomposition onset at 444 °C (47% weight loss at 500 °C)

Source: Huntsman 2002.

Test substance: C10-14 Monoalkylbenzene sulfonic acid, sodium salt (CAS

> #85117-50-6); mean molecular weight = 348, average alkyl chain length = C12.0. The test material is 85% active matter and is

a coarse, cream-colored powder at 25°C.

Reliability: (2) valid with restrictions

21-FEB-2003 (23)

2.2 Boiling Point

= 156 degree C Value:

GLP: no

Source: CONDEA Vista 1995.

Test substance: Alkylbenzene sulfonic acid with the following composition:

Components	CAS Number	Weight%
Nonylbenzenesulfonic Acid	35298-13-6	0.6
n-Decylbenzenesulfonic Acid	140-60-3	18.3
Undecylbenzenesulfonic Acid	50854-94-9	42.1
Dodecylbenzenesulfonic Acid	27176-87-0	30.0
Tridecylbenzenesulfonic Acid	25496-01-9	4.4
Tetradecylbenzenesulfonic Ac	id 30776-59-1	0.5
Sulfuric Acid	7664-93-9	1.3
Free Oil	None	2.4
Water	7732-18-5	0.4

(4) not assignable Reliability:

Data from Material Safety Data Sheet. No report available for

review.

21-FEB-2003 (4)

Value: = 315 degree C

no data GLP:

Verschueren 1996. Source:

Test substance: Benzene sulfonic acid, dodecyl- (27176-87-0)

Reliability: (2) valid with restrictions Peer-reviewed reference book.

21-FEB-2003 (80)

- 7/55 -

= 205 degree C at 1013 hPa Value:

Decomposition: no

GLP: no data
mark: IUCLID cites source as Hoecht Iberica s.a. Barcelona.
urce: IUCLID 1995. Remark:

Source:

Test substance: Benzene sulfonic acid, dodecyl- (27176-87-0)

Reliability: (2) valid with restrictions

21-FEB-2003 (28)

Value:

Decomposition: yes

Method: other: Thermal analysis was performed on the Netzsch DSC 204C

and TG209C with N2 atmosphere.

GLP:

Decomposition onset at 444°C (47% weight loss at 500°C) Remark:

Huntsman 2002. Source:

Test substance: C10-14 monoalkylbenzene sulfonic acid, sodium salt (CAS

#85117-50-6); mean molecular weight = 348, average alkyl chain length = C12.0. The test material is 85% active matter and is

a coarse, cream-colored powder at 25°C.

(2) valid with restrictions Reliability:

21-FEB-2003 (23)

2.3 Density

Type: Value:

Not an HPV Challenge endpoint. Remark:

21-MAR-2003

2.3.1 Granulometry

Type of

distribution:

Remark: Not an HPV Challenge endpoint.

21-MAR-2003

- 8/55 -

2.4 Vapour Pressure

= .22 hPaValue:

GLP: no

Source: CONDEA Vista 1995.

Test substance: Alkylbenzene sulfonic acid with the following composition:

Components	CAS Number	Weight%
Nonylbenzenesulfonic Acid n-Decylbenzenesulfonic Acid Undecylbenzenesulfonic Acid Dodecylbenzenesulfonic Acid Tridecylbenzenesulfonic Acid Tetradecylbenzenesulfonic Acid Sulfuric Acid Free Oil Water	35298-13-6 140-60-3 50854-94-9 27176-87-0 25496-01-9 30776-59-1 7664-93-9 None 7732-18-5	0.6 18.3 42.1 30.0 4.4 0.5 1.3 2.4
	10 0	J • 1

Reliability: (4) not assignable

Data from Material Safety Data Sheet. No report available for

review.

21-FEB-2003 (4)

Value: = 0 hPa

Method: other (calculated)

The reported value is 3x10-13 Pa.

Cites estimates calculated by Lyman (see References).

HERA 2002; Lyman 1985. Source: **Test substance:** C12 LAS (CAS #25155-30-0) Reliability: (4) not assignable

(18) (43)21-FEB-2003

2.5 Partition Coefficient

= 2 at 23 degree C log Pow:

OECD Guide-line 107 "Partition Coefficient (n-octanol/water), Method:

Flask-shaking Method"

1981 Year: GLP: no

Remark: IUCLID cites source as Shell Chemical U.K. Ltd. Chester. No

report available for review.

IUCLID 1995. Source:

Test substance: Benzene sulfonic acid, C10-16-alkyl derivatives (68584-22-5)

Reliability: (2) valid with restrictions

05-DEC-2001 (27)

- 9/55 -

2. Physico-chemical Data

log Pow: = 1.96

Method: other (calculated): Leo and Hansch

Year: 1971 GLP: no data

Remark: Original data from Leo, A., Hansch, C., and Elkins, D. 1971.

Chem. Rev. 71:525-616.

Hand and Williams 1987. Source:

Test substance: Sodium dodecylbenzenesulfonate as a surrogate for benzene

sulfonic acid, dodecyl- (27176-87-0)

Reliability: (2) valid with restrictions

Based on data from standard reference source.

11-OCT-2001 (16)

log Pow: = 2.52

Method: other (calculated): Leo and Hansch

Year: 1971 GLP: no data

Original data from Leo, A., Hansch, C., and Elkins, D. 1971. Remark:

Chem. Rev. 71:525-616.

Hand and Williams 1987. Source:

Test substance: Sodium tridecylbenzene sulfonate as surrogate for benzene

sulfonic acid, tridecyl- (25496-01-9)

Reliability: (2) valid with restrictions

Based on data from standard reference source.

11-OCT-2001 (16)

log Pow: = 3.32

Method: other (calculated)

Year:

GT.P: no

Remark: Calculated using the method of Leo and Hansch (1979) modified

to take into account the various phenyl positions along the

linear alkyl chain as per Roberts (1991).

Source: HERA 2002; Roberts 1991; Leo and Hansch 1979.

Test substance: C11.6 LAS

Reliability: (4) not assignable

21-FEB-2003 (18) (39) (65)

2.6.1 Water Solubility

400000 mg/l at 20 degree C Value:

GLP:

The IUCLID Data Sheet cites a Shell Chemical report indicating Remark:

that the substance is miscible in water up to 40%.

Source: IUCLID 1995.

Test substance: Benzene sulfonic acid, C10-16-alkyl derivatives (68584-22-5)

Reliability: (2) valid with restrictions

05-DEC-2001 (27)

-10/55 -

2. Physico-chemical Data

= 300000 mg/l at 20 degree C Value:

> 9 pH: GLP: no data

Remark: The IUCLID Data Sheet cites a Shell Chemical report indicating

that the substance is miscible in water up to 40%.

Source: IUCLID 1995.

Test substance: Benzene sulfonic acid, dodecyl- (27176-87-0)

Reliability: (2) valid with restrictions

04-DEC-2001 (28)

Result: The reported pKa for all of the LAB sulfonic acids is < 1.

Noeller 1966; Lide 1990. Source:

Test substance: Benzene sulfonic acid, C10-16-alkyl derivatives (68584-22-5),

Benzene sulfonic acid, dodecyl- (27176-87-0), and Benzene

sulfonic acid, tridecyl- (25496-01-9)

(2) valid with restrictions Reliability:

11-OCT-2001 (40) (50)

Value: > 250 q/1Qualitative: miscible no data GLP:

Remark: The study shows that 25% solutions (250 g/L) of various LASs

> have cloud clear points (i.e., form clear solutions) at temperatures of 2-21°C or above. Therefore, the results demonstrate that 25% solutions of LAS are soluble at room

temperature.

Source: Cohen 1995.

Test substance: Various LASs made from four commercial LABs, average alkyl

chain length = 11.6

Reliability: (2) valid with restrictions

21-FEB-2003 (3)

= 10 GLP: no data

Reported pH value is 10.0 +/- 1.0 (1% solution). Remark:

Source: Huntsman 2002.

Test substance: C10-14 monoalkylbenzene sulfonic acid, sodium salt (CAS

#85117-50-6); mean molecular weight = 348, average alkyl chain

length = C12.0

Reliability: (4) not assignable

21-FEB-2003 (22)

2.6.2 Surface Tension

Not an HPV Challenge endpoint. Remark:

20-FEB-2003

- 11/55 -

2.7 Flash Point

Value: Type: Method: Year:

Remark: Not an HPV Challenge endpoint.

20-FEB-2003

2.8 Auto Flammability

Value:

Remark: Not an HPV Challenge endpoint.

20-FEB-2003

2.9 Flammability

Result:

Remark: Not an HPV Challenge endpoint.

20-FEB-2003

2.10 Explosive Properties

Result:

Remark: Not an HPV Challenge endpoint.

20-FEB-2003

2.11 Oxidizing Properties

Result:

Remark: Not an HPV Challenge endpoint.

20-FEB-2003

2.12 Additional Remarks

Memo: None

11-OCT-2001

- 12/55 -

3.1.1 Photodegradation

Type: air INDIRECT PHOTOLYSIS Sensitizer:

Conc. of sens.: 1500000 molecule/cm3

Rate constant: = .00000000001352 cm3/(molecule * sec)

Degradation: = 50 % after 8.6 hour(s)

Method: other (calculated): EPISuite, Version 3.10

Year: GLP:

Test substance:

USEPA 2000. Source:

Test substance: Benzene sulfonic acid, undecyl (50854-94-9) as a surrogate for

Benzene sulfonic acid, C10-16-alkyl derivatives (68584-22-5).

The C11 sulfonic acid was used because it more closely approximates the average alkyl chain length for the C10-16 material, which ranges from 11.0 to 11.8. The EpiSuite model calculates the C10-16 material based on its lowest alkyl chain length, which is C10. This half-life value was 9.5 hours.

Reliability: (2) valid with restrictions

Standard peer-reviewed database and estimation software.

21-JAN-2002 (76)

Type: air INDIRECT PHOTOLYSIS Sensitizer:

Conc. of sens.: 1500000 molecule/cm3

Rate constant: = .00000000001636 cm3/(molecule * sec)

Degradation: = 50 % after 7.9 hour(s)

Method: other (calculated): EPISuite, Version 3.10

Year: GLP:

Test substance: other TS: Benzene sulfonic acid, dodecyl (27176-87-0). The

EPISuite model calculates this material based on a C12 alkyl chain length rather than the full range of carbon chain

lengths present.

Source: USEPA 2000.

Reliability: (2) valid with restrictions

Standard peer-reviewed database and estimation software.

21-JAN-2002 (76)

- 13/55 -

3. Environmental Fate and Pathways

Type: INDIRECT PHOTOLYSIS OH Sensitizer:

Conc. of sens.: 1500000 molecule/cm3

Rate constant: = .00000000001777 cm3/(molecule * sec)

Degradation: = 50 % after 7.2 hour(s)

Method: other (calculated): EPISuite, Version 3.10

GLP: Year:

Test substance: other TS: Benzene sulfonic acid, tridecyl (25496-01-9). The

EPISuite model calculates this material based on a C13 alkyl chain length rather than the full range of carbon chain

lengths present.

Source: USEPA 2000.

Reliability: (2) valid with restrictions

Standard peer-reviewed database and estimation software.

21-JAN-2002 (76)

Type: air INDIRECT PHOTOLYSIS Sensitizer: \cap H

Conc. of sens.: 1500000 molecule/cm3

Rate constant: = .00000000001339 cm3/(molecule * sec)

Degradation: = 50 % after 7.9 hour(s)

other (calculated): EPISuite, Version 3.10 Method:

Year:

Test substance: other TS: Linear Alkylbenzene Sulfonate (LAS) (25155-30-0 et

al.). The modeled material was a C12-LAS.

USEPA 2000. Source:

Reliability: (2) valid with restrictions

Standard peer-reviewed database and estimation software.

21-JAN-2002 (76)

Type: water

Light source: other: Mercury vapor lamp

= 200 - 350 nmLight spect.:

DIRECT PHOTOLYSIS

> 95 % after 20 minute(s) Degradation:

Method:

Year: GLP: no data

Test substance: other TS: LAS; activity: 95% (CAS #25155-30-0)

Method:

A series of photodegradation studies were conducted. Aqueous solution of LAS (pH 6.75) were passed through an irradiated tubular flow reactor. Reaction rates were obtained for both non-sensitized conditions and when ferric perchlorate (0.04 to $3.15 \times 10-4 \text{ q-mole/L})$ was used as a sensitizer. A Hanovia 1200-watt mercury-vapor lamp was the source of radiation. The LAS concentration was determined by the methylene blue method.

Rapid photodegradation occurred in indirect photolysis Remark:

degradation. Complete conversion of LAS to intermediates at an average residence time as low as 1 minute. The maximum conversion to CO2 was obtained at a residence time of 20 minutes and corresponded to 7 moles CO2 per mole of LAS.

Reaction rate increases by two orders of magnitude in presence of ferric perchlorate. Half order kinetics with respect to

- 14/55 -

light intensity and LAS concentration explained the data for nonsensitized conditions. An appropriate rate equation could

be derived by assuming a second-order deactivation of

light-activated LAS molecules. The sensitized reaction was believed to occur by abstraction of hydrogen atoms from LAS by hydroxyl radicals. Hydroxyl radicals presumably are produced by an electron-transfer reaction involving light-activated ferric ions. The mechanism is complex; over-all kinetics indicated a first-order effect of (Fe+3), 1.2 order in light intensity, and maxima in the rate for intermediate LAS and O2

concentrations.

Initial LAS concentration was 60 to 182 mg/L.

Source: Matsuura and Smith 1970. (2) valid with restrictions Reliability:

20-FEB-2003 (45)

3.1.2 Stability in Water

Type: abiotic

Method:

GLP: no data Year:

Test substance: other TS: C10-13 alkylbenzene sulfonic acid, sodium salt (CAS

#68411-30-3)

LAS is stable in water. LAS can be decomposed at extreme Remark:

conditions such as elevated temperatures in the presence of inorganic acids such as phosphoric, sulphuric and hydrochloric acid, e.g.: 60-70% sulphuric acid at 140 - 190 degree C or with concentrated HCl in a sealed container at 150 - 200 degree C. Information as cited in IUCLID Data Sheet for CAS

#68411-30-3.

Cross and Dekker 1977. Source: (4) not assignable Reliability:

21-FEB-2003 (5)

3.1.3 Stability in Soil

Radiolabel: Type:

Concentration: Cation exch. capac. Microbial biomass: Method:

> Year: GLP:

Test substance:

Remark: Not an HPV Challenge endpoint.

20-FEB-2003

- 15/55 -

3.2 Monitoring Data (Environment)

Type of

measurement:

Medium:

Remark: None

02-NOV-2001

3.3.1 Transport between Environmental Compartments

Type: Media: Method: Year:

Remark: Not an HPV Challenge endpoint.

20-FEB-2003

3.3.2 Distribution

Media:

Method: other (calculation): Fugacity Level III

Year:

Mass Distribution by Environmental Compartment Remark:

> Air: 1.13% Water: 31.7% Soil: 63.3% Sediment: 3.81%

USEPA 2000. Source:

Test substance: Benzene sulfonic acid, undecyl (50854-94-9), which best

represents the actual alkyl chain length (11.0-11.8) of Benzene sulfonic acid, C10-16 alkyl derivatives (68584-22-5)

Reliability: (2) valid with restrictions

21-JAN-2002 (76)

Media:

other (calculation): Fugacity Level III Method:

Year:

Remark: Mass Distribution by Environmental Compartment

> Air: 1.03% Water: 29.1% 59.7% Soil: Sediment: 10.0%

Source: USEPA 2000.

Test substance: Benzene sulfonic acid, dodecyl- (27176-87-0)

Reliability: (2) valid with restrictions

02-NOV-2001 (76)

3. Environmental Fate and Pathways

Media:

other (calculation): Fugacity Level III Method:

Year:

Remark: Mass Distribution by Environmental Compartment

> Air: 0.878% 23.3% Water: Soil: 52.4% Sediment: 23.4%

USEPA 2000. Source:

Test substance: Benzene sulfonic acid, tridecyl- (25496-01-9)

Reliability: (2) valid with restrictions

02-NOV-2001 (76)

Media:

Method: other (calculation): Fugacity Level III

Year:

Remark: Mass Distribution by Environmental Compartment

> 1.14% Air: Water: 34.1% 64.4% Soil: Sediment: 0.367%

USEPA 2000.

Test substance: Linear Alkylbenzene Sulfonate (LAS) (25155-30-0 et al.) (The

modeled material was a C12-LAS)

Reliability: (2) valid with restrictions

20-FEB-2003 (76)

3.4 Mode of Degradation in Actual Use

The LAB sulfonic acids are intermediates in the production of Memo:

LAS.

11-OCT-2001

- 17/55 -

3.5 Biodegradation

Type: aerobic

Inoculum: activated sludge

Concentration: 11.3 mg/l related to DOC (Dissolved Organic Carbon)

Contact time: 28 day

Degradation: = 94 % after 28 day readily biodegradable Result:

Method: other: OECD DOC-Die away test (EG - Richtlinie 92/69 EWG, Tiel

II, C.4-A)

Year: 1992 **GLP:** yes

Test substance: other TS: Benzenesulfonic acid, C10-13-alkyl derivatives (85536-14-7) as a surrogate for benzene sulfonic acid,

C10-16-alkyl derivatives (68584-22-5)

Kurtin 1994. Source:

Reliability: (1) valid without restriction

05-DEC-2001 (33)

Type: aerobic

Inoculum: domestic sewage

Concentration: 11.6 mg/l related to Test substance
Contact time: 37 day
Degradation: = 92 % after 37 day

Method: other: Modified coupled units test Year: 1991 GLP: yes

Test substance: other TS: Benzenesulfonic acid, C10-13-alkyl derivatives

(85536-14-7) as a surrogate for benzene sulfonic acid,

C10-16-alkyl derivatives (68584-22-5)

Kurtin 1994; Schoberl 1991. Source: Reliability: (1) valid without restriction

04-DEC-2001 (34) (67)

aerobic Type:

Inoculum: activated sludge

20 mg/l related to DOC (Dissolved Organic Carbon)

Contact time: 28 day
Degradation: = 69 % after 28 day

Method: OECD Guide-line 301 B "Ready Biodegradability: Modified Sturm

Test (CO2 evolution)"

1992 Year: GLP: no data

Test substance: other TS: Benzene sulfonic acid, dodecyl- (27176-87-0)

Remark: % degradation refers to mineralization.

Stepan; OECD 1992. Source:

Reliability: (2) valid with restrictions

03-JUL-2001 (61) (69)

- 18/55 -

3. Environmental Fate and Pathways

Type: aerobic

activated sludge, domestic, non-adapted Inoculum:

10.8 mg/l related to DOC (Dissolved Organic Carbon) Concentration: 10.8 mg
Contact time: 28 day
Degradation: = 93 %

Degradation: = 93 % after 28 day Result: readily biodegradable Kinetic: 7 day = 59 %14 day = 73 % 21 day = 82 %

other: Directive 79/831/EEC, Appendix V, C.4-A. DOC Die-Away Method:

Test

GLP: yes Year: 1990

Test substance: other TS: Linear Alkylbenzene Sulfonate (LAS) (68411-30-3 et

Remark: The many biodegradation studies for LAS all report that LAS is

readily biodegradable.

Huels 1993. Source:

Reliability: (2) valid with restrictions

11-OCT-2001 (21)

3.6 BOD5, COD or BOD5/COD Ratio

Remark: Not an HPV Challenge endpoint.

21-MAR-2003

3.7 Bioaccumulation

Leuciscus idus melanotus (Fish, fresh water) Species:

Exposure period: 3 day

Concentration:

BCF: = 130

Elimination:

Method: other: Golden ide were exposed to a constant water

concentration of the dissolved test material for 3 days.

GLP: no

Test substance: other TS: Dodecylbenzenesulphate sodium salt as a surrogate

for benzene sulfonic acid, dodecyl- (27176-87-0)

Remark: A BCF of 130 indicates a moderate affinity for uptake in fish

tissues. However, uptake into tissues may be offset by

metabolism and/or excretion.

Freitag et al. 1985. Source:

(1) valid without restriction Reliability:

11-OCT-2001 (14)

- 19/55 -

3. Environmental Fate and Pathways

Pimephales promelas (Fish, fresh water) Species:

Exposure period: 48 hour(s)

2.7 Concentration:

BCF: = 22 - 87

Elimination: yes

OECD Guide-line 305 E "Bioaccumulation: Flow-through Fish Method:

Test"

1981 Year: **GLP:** yes

Test substance: other TS: LAS (C10-13), tested individually and as mixtures,

activity: >97.4%

Method: The exposure phase in Experiment A was 48-hours. The exposure

> phase in Experiments B-D ranged from 168 to 192 hours. Fish were then transferred to untreated water for the depuration

Remark: BCF values ranged between 2-1000 L/kg with BCFs increasing

with increasing alkyl chain length. To address differences in

composition of mixtures, bioconcentration potential was evaluated for a mixture typical of LAS in European detergent formulations (C10 12%, C11 29%, C12 34%, C13 24%; average alkyl chain length = C11.6) and a mixture typical of LAS in filtered Mississippi river water (C10 45%, C11 23%, C12 23%, C13 2%; average chain length = C10.8). The respective BCFs were 87 and 22 L/kg at concentrations of 2.7 and 4.1 uM, indicating that environmental processes decrease the

bioconcentration potential of LAS.

Tolls 1997; OECD 1981. Source:

Test condition: The type of test was measured and flow-through.

(2) valid with restrictions Reliability:

20-FEB-2003 (51) (74)

3.8 Additional Remarks

Memo: None

02-NOV-2001

-20/55 -

AQUATIC ORGANISMS

4.1 Acute/Prolonged Toxicity to Fish

Type: flow through

Species: Cyprinus carpio (Fish, fresh water)

Exposure period: 96 hour(s)

Unit: mq/l Analytical monitoring:

LC50: = 5.6

Method: OECD Guide-line 203 "Fish, Acute Toxicity Test"
Year: 1984 GLP: yes

Test substance: other TS: Benzenesulfonic acid, C10-13-alkyl derivatives

(85536-14-7) as a surrogate for benzene sulfonic acid,

C10-16-alkyl derivatives (68584-22-5)

Remark: The LCO and LC100 were 4 and 8 mg/L, respectively.

Source: Kurtin 1997; OECD 1984.

Reliability: (1) valid without restriction

02-JUL-2001 (36)

Type: static

Species: Leuciscus idus (Fish, fresh water)

Exposure period: 96 hour(s)

Unit: mg/l Analytical monitoring: no

LC0: = 4 LC50: = 4.1 LC100: = 4.3

Method: other: DIN 38412 Part 15

Year: GLP: yes

Test substance: other TS: n-dodecylbenzenesulfonate as a surrogate for benzene

sulfonic acid dodecyl- (27176-87-0)

Source: Knie et al. 1983

Reliability: (1) valid without restriction

03-JUL-2001 (7) (30)

Type: static

Species: Brachydanio rerio (Fish, fresh water)

Exposure period: 96 hour(s)

Unit: mg/l Analytical monitoring: no

LC50: = 10

Method: OECD Guide-line 203 "Fish, Acute Toxicity Test"
Year: 1992 GLP: yes

Test substance: other TS: Dodecylbenzenesulfonate-sodium salt as a surrogate

for benzene sulfonic acid, dodecyl- (27176-87-0)

Source: OECD 1992; IUCLID 1995.
Reliability: (2) valid with restrictions

Company GLP report cited in IUCLID Data Sheet but not

available for review.

03-JUL-2001 (19)

- 21/55 -

Type: other: daily renewal

Species: Salmo gairdneri (Fish, estuary, fresh water)

Exposure period: 96 hour(s)

Unit: mg/l Analytical monitoring: no

LC50: = 4.3

Method: OECD Guide-line 203 "Fish, Acute Toxicity Test"
Year: 1992 GLP: no

Test substance: other TS: Benzene sulfonic acid, dodecyl- (27176-87-0)

LC50 is geometric mean of lower (3.2 mg/L) and upper (5.6 mg/L) limits from a series of studies investigating the reduction in number of individuals needed for testing.

Source: OECD 1992; Douglas et al. 1986. Reliability: (1) valid without restriction

03-JUL-2001 (10) (60)

Type: static

Species: Salmo gairdneri (Fish, estuary, fresh water)

Exposure period: 96 hour(s)

Unit: mg/l Analytical monitoring: yes

LC50: = 3

Method:

Year: 1981 **GLP:** yes

Test substance: other TS: Dobanic acid 102 (linear alkyl benzenesulfonic acid,

C10-13) as a surrogate for Benzene sulfonic acid, tridecyl-

(25496 - 01 - 9)

Method: Five aquaria were filled with a series of concentrations

between 0.2 and 5 mg/l of Dobanic acid 102. One aquarium was a control. Five fish were placed in each aquarium. The concentration, temperature, and pH were kept constant.

Source: Stephenson 1981.

Reliability: (1) valid without restriction

03-JUL-2001 (70)

Type: semistatic

Species: Salmo gairdneri (Fish, estuary, fresh water)

Exposure period: 96 hour(s)

Unit: mg/l Analytical monitoring: yes

LC50: = 5.8

Method: OECD Guide-line 203 "Fish, Acute Toxicity Test"
Year: 1992 GLP: no data

Test substance: other TS: Linear Alkylbenzene Sulfonate (LAS) (68411-30-3 et

al.)

Remark: Analysis showed 92% of nominal concentration, tap water, water

hardness; 96-120 mg/L CaCO3, pH 6.8-7.3, daily renewal,

14.5-16 C; life-stage: 5 months.

Source: Procter & Gamble 1991; OECD 1992.
Reliability: (1) valid without restriction

11-OCT-2001 (60) (63)

- 22/55 -

Type:

Species: Lepomis macrochirus (Fish, fresh water)

Exposure period:

Unit: mg/l Analytical monitoring:

LC50: = 3

Method:

Year: GLP:

Test substance: other TS: LAS normalized to C11.6

Remark: Mean LC50 for bluegill sunfish was derived from a total of 88

records compiled from several literature reviews.

Source: van de Plassche et al. 1999.

Reliability: (4) not assignable

21-FEB-2003 (77)

Type:

Species: Pimephales promelas (Fish, fresh water)

Exposure period:

Unit: mg/l Analytical monitoring:

LC50: = 3.2

Method:

Source:

Year: GLP:

Test substance: other TS: LAS normalized to C11.6

Remark: Mean LC50 for fathead minnow was derived from a total of 35

records compiled from several literature reviews.

Source: van de Plassche et al. 1999.

Reliability: (4) not assignable

21-FEB-2003 (77)

4.2 Acute Toxicity to Aquatic Invertebrates

Species: Daphnia magna (Crustacea)

Exposure period: 48 hour(s)

Unit: mg/l Analytical monitoring: yes

EC50: = 5.2

Method: OECD Guide-line 202, part 1 "Daphnia sp., Acute

Immobilisation Test"

Year: 1984 GLP: yes

Test substance: other TS: 4-C10-13 Alkylbenzene sulfonic acid (85536-14-7) as

a surrogate for benzene sulfonic acid, C10-16-alkyl

derivatives (68584-22-5) Kurtin 1995; OECD 1984.

Reliability: (1) valid without restriction

21-FEB-2003 (35) (62)

- 23/55 -

Species: Daphnia magna (Crustacea)

Exposure period: 48 hour(s)

Unit: mg/l Analytical monitoring: no data

EC50: = 9.3 - 11.6

Method: OECD Guide-line 202, part 1 "Daphnia sp., Acute

Immobilisation Test"

Year: 1984 GLP: yes

Test substance: other TS: See Remark

Remark: The toxicity values of the LAB sulfonic acids are in the same

order as their sodium salts. As the chain length gets longer, the LC50 decreases. Three LAB sulfonic acids of varying chain lengths neutralized with caustic soda to obtain the sodium salt derivative were tested. Acid A had 48.4% of its weight in the C11 range and the majority its chain length ranged from C10-C13. Acid B had 49.4% of its weight in the C11 range and 31.7% of its weight in the C12 range. The majority of its chain length ranged from C10 to C12. Acid C had the majority of its chain length in the C10 to C13 range, almost evenly

distributed between C11 and C12.

Result: Acid A had a LC50 of 11.6 mg/L, acid B 10.8 mg/L, and acid C

9.3 mg/L.

Source: Verge 2000; OECD 1984.

Reliability: (1) valid without restriction

21-FEB-2003 (57) (79)

Species: Daphnia magna (Crustacea)

Exposure period: 48 hour(s)

Unit: mg/l Analytical monitoring: no

EC50: = 2.9

Method: other: The test solution was added to dishes in concentrations

ranging from 0.3-20~mg/l with controls. Ten organisms were added to each dish. Immobilised organisms were recorded at 24

and 48 hours.

Year: 1981 GLP: yes

Test substance: other TS: Dobanic acid (linear alkyl benzenesulfonic acid,

C10-13) as a surrogate for benzene sulfonic acid, C10-16-alkyl

derivatives (68584-22-5)

Source: Stephenson 1981.

Reliability: (1) valid without restriction

21-FEB-2003 (70)

- 24/55 -

Daphnia magna (Crustacea)

Exposure period: 24 hour(s)

Unit: mg/l Analytical monitoring: no

EC0: = 6 EC50: = 12 = 14 EC100:

Method: other: DIN 38412 Part 11

Year: **GLP:** yes

Test substance: other TS: n-dodecylbenzenesulfonate as a surrogate for benzene

sulfonic acid, dodecyl- (27176-87-0)

Source: Knie et al. 1983.

Reliability: (1) valid without restriction

20-FEB-2003 (6) (30)

Species: Daphnia magna (Crustacea)

Exposure period: 48 hour(s)

mg/l Analytical monitoring: yes

EC50: = 5.88

Method: Directive 84/449/EEC, C.2 "Acute toxicity for Daphnia"

Year: GLP: no data

Test substance: other TS: Benzene sulfonic acid, dodecyl- (27176-87-0)

Source: Galassi et al. 1992; EEC Directive.

Reliability: (2) valid with restrictions

Data as cited in IUCLID data sheet.

20-FEB-2003 (9) (15)

Species: Daphnia magna (Crustacea)

Exposure period: 48 hour(s)

Unit: mg/l Analytical monitoring: no data

EC50: = 4.3

Method: OECD Guide-line 202, part 1 "Daphnia sp., Acute

Immobilisation Test"

Year: 1984 GLP: yes

Test substance:

Verge et al. 2000; OECD 1984.

Test substance: The substance tested was derived from a LAB product with 67.0%

of its weight in the C13 range. The rest of the weight is spread over the C10-C14 range. Used as a surrogate for

benzene sulfonic acid, tridecyl- (25496-01-9).

Reliability: (1) valid without restriction

21-FEB-2003 (57) (79)

Daphnia magna (Crustacea) Species:

Exposure period: 48 hour(s)

Unit: mq/1Analytical monitoring: no

EC50: = 6.8

Directive 84/449/EEC, C.2 "Acute toxicity for Daphnia" Method:

1984 GLP: yes Year:

Test substance: other TS: Linear Alkylbenzene Sulfonate (LAS) (68411-30-3 et

al.)

EEC Directive 1984. Source:

Reliability: (1) valid without restriction

21-FEB-2003 (9)

- 25/55 -

Species: Daphnia magna (Crustacea)

Exposure period:

Unit: mg/l Analytical monitoring:

EC50: = 4.1

Method:

Year: GLP:

Test substance: other TS: C10-13 LAS (CAS #68411-30-3)

Remark: D. magna was selected as the representative test organism of

the toxicity of LAS to invertebrates. The value is a mean of 17 records of commercially representative LAS with C10-13 alkyl chain lengths and average carbon numbers of C11.6 and

C11.8.

Source: HERA 2002.

Reliability: (4) not assignable

21-FEB-2003 (18)

Species: Daphnia magna (Crustacea)

Exposure period:

Unit: mg/l Analytical monitoring:

EC50: = 4.7

Method:

Year: GLP:

Test substance: other TS: LAS normalized to C11.6

Remark: EC50 is geometric mean of 139 records compiled from literature

reviews. Values range from 0.26 to 55 mg/L. This large range is caused by differences in the LAS tested with respect to alkyl chain and/or phenyl isomer distribution and differences

in test design.

Source: van de Plassche et al. 1999.

Reliability: (4) not assignable

21-FEB-2003 (77)

4.3 Toxicity to Aquatic Plants e.g. Algae

Species: Scenedesmus subspicatus (Algae)

Unit: mg/l Analytical monitoring: yes

EC50: = 36

Method: OECD Guide-line 201 "Algae, Growth Inhibition Test"
Year: 1984 GLP: yes

Test substance: other TS: Benzenesulfonic acid, C10-13-alkyl derivatives

(85536-14-7) as a surrogate for benzene sulfonic acid,

C10-16-alkyl derivatives (68584-22-5)

Remark: The reported EC50 is for growth rate. The 72-hr EC50 for

biomass was also tested in this experiment and determined to

be 14 mg/L for this substance.

Source: Kurtin 1994; OECD 1984.

Reliability: (1) valid without restriction

21-FEB-2003 (32) (56)

- 26/55 -

Species: Selenastrum capricornutum (Algae)

Endpoint: growth rate

Exposure period: 4 day

Unit: mg/l Analytical monitoring: no

EC50: = 170

Method: other: Twelve flasks were filled with quanities of test

solution ranging from 2--200~mg/l. Six flasks served as controls. Algae was added to each container. Cell counts

were made after 2 and 4 days.

Year: 1981 **GLP:** yes

Test substance: other TS: Dobanic acid (linear alkyl benzenesulfonic acid,

C10-13) as a surrogate for benzene sulfonic acid, C10-16-alkyl

derivatives (68584-22-5)

Source: Stephenson 1981.

Reliability: (1) valid without restriction

21-FEB-2003 (70)

Species: Haematococcus pluvialis (Algae)
Endpoint: other: inhibition of oxygen production

Exposure period: 4 hour(s)

Unit: mg/l Analytical monitoring: no

EC50: = 50

Method: other: Based on the procedure by Tumpling. The initial cell

density was 80,000 cells/mL.

Year: GLP: yes

Test substance: other TS: n-dodecylbenzenesulfonate as a surrogate for benzene

sulfonic acid, dodecyl- (27176-87-0)

Source: Knie et al. 1983.

Reliability: (1) valid without restriction

20-FEB-2003 (30)

Species: Selenastrum capricornutum (Algae)

Endpoint: growth rate
Exposure period: 96 hour(s)

Unit: mg/l Analytical monitoring: yes

EC50: = 29

Method: other: EPA method

Year: 1985 **GLP:** no

Test substance: other TS: Benzene sulfonic acid, dodecyl- (27176-87-0)

Source: Galassi et al. 1992; EPA 1985.
Reliability: (2) valid with restrictions

Data as cited in IUCLID data sheet.

20-FEB-2003 (15) (75)

- 27/55 -

Species: Scenedesmus subspicatus (Algae)

Endpoint: growth rate
Exposure period: 72 hour(s)

Unit: mg/l Analytical monitoring: no

NOEC: = 30 **EC50:** = 163

Method: OECD Guide-line 201 "Algae, Growth Inhibition Test"
Year: 1984 GLP: no data

Test substance: other TS: Linear Alkylbenzene Sulfonate (LAS) (68411-30-3 et

al.)

Source: Verge 1996; OECD 1984.

Reliability: (2) valid with restrictions

21-FEB-2003 (56) (78)

Species: Endpoint:

Exposure period:

Unit: mg/l Analytical monitoring:

1C50 : = 9.1

Method:

Year: GLP:

Test substance: other TS: C10-13 LAS (CAS #68411-30-30)

Remark: Data are for various algae species. The value is a geometric

mean of 12 records of commercially representative LAS with ${\rm C10-13}$ alkyl chain lengths and average carbon number of ${\rm C11.6}$

and C11.8.

Source: HERA 2002.

Reliability: (4) not assignable

21-FEB-2003 (18)

4.4 Toxicity to Microorganisms e.g. Bacteria

Type: Species:

Exposure period:

Unit: Analytical monitoring:

Method:

Year: GLP:

Test substance:

Remark: Not an HPV Challenge endpoint.

21-MAR-2003

- 28/55 -

4.5 Chronic Toxicity to Aquatic Organisms

4.5.1 Chronic Toxicity to Fish

Species: other: Brachydanio rerio, Pimephales promelas, Poecilia

reticulata, Oncorhynchus mykiss, and Tilapia mossambica

Endpoint: other: growth

Exposure period: 28 day

Unit: mg/l Analytical monitoring: no

NOEC: = .25 - 3.2

Method:

Year: GLP: no data

Test substance: other TS: Linear Alkylbenzene Sulfonate (LAS) (68411-30-3 et

al.)

Remark: All data were from tests conducted on commercial LAS with

C10-13 alkyl chains and average carbon lengths of C11.6 and C11.8. The NOEC values have been normalized using QSARs to

the average structure of C11.6 LAS.

Result: The article compiles the no observed effect concentration

(NOEC) values for many tests conducted on an assortment of species. The following table shows the geometric mean NOEC values for each fish species (n = number of studies included

for each species).

Species Geometric mean NOEC (mg/L) n

Brachydanio rerio 2.3 1
Pimephales promelas 0.87 14
Poecilia reticulata 3.2 1
Oncorhynchus mykiss 0.34 7
Tilapia mossambica 0.25 1

Source: van de Plassche et al. 1999.

Reliability: (4) not assignable

21-MAR-20 (77)

03

4.5.2 Chronic Toxicity to Aquatic Invertebrates

Species: Daphnia magna (Crustacea)

Endpoint:

Exposure period:

Unit: mg/l Analytical monitoring:

NOEC: = 1.4

Method:

Year: GLP:

Test substance: other TS: LAS normalized to C11.6

Remark: NOEC is geometric mean of 12 records compiled from literature

reviews and normalized to C11.6.

Source: van de Plassche et al. 1999.

Reliability: (4) not assignable

21-FEB-2003 (77)

TERRESTRIAL ORGANISMS

4.6.1 Toxicity to Soil Dwelling Organisms

Type: Species: Endpoint:

Exposure period:

Unit: Method:

Year: GLP:

Test substance:

Remark: Not an HPV Challenge endpoint.

20-FEB-20

03

4.6.2 Toxicity to Terrestrial Plants

Species: Endpoint:

Expos. period:

Unit: Method:

Year: GLP:

Test substance:

Remark: Not an HPV Challenge endpoint.

20-FEB-2003

4.6.3 Toxicity to other Non-Mamm. Terrestrial Species

Species: Endpoint:

Expos. period:
Unit:

Method:

Year: GLP:

Test substance:

Remark: Not an HPV Challenge endpoint.

20-FEB-2003

4.7 Biological Effects Monitoring

Memo: Not an HPV Challenge endpoint.

20-FEB-2003

4.8 Biotransformation and Kinetics

Type:

Remark: Not an HPV Challenge endpoint.

20-FEB-2003

4.9 Additional Remarks

Memo: None

11-OCT-2001

- 31/55 -

5.1 Acute Toxicity

5.1.1 Acute Oral Toxicity

Type: LD50

Species: other: rat, Wistar

Sex: male/female

Number of

Animals: 10

Vehicle: other: none
Value: = 1470 mg/kg bw

Method: OECD Guide-line 401 "Acute Oral Toxicity"
Year: 1981 GLP: yes

Test substance: other TS: Benzenesulfonic acid, C10-13-alkyl derivatives

(85536-14-7) as a surrogate for benzene sulfonic acid,

C10-16-alkyl derivatives (68584-22-5)

Remark: Five of each sex per dose level were tested. Test duration

was 14 days. The dose range was 1250-1990 mg/kg.

Source: Murmann 1984; OECD 1981.

Reliability: (1) valid without restriction

21-FEB-2003 (46) (52)

Type: LD50

Species: other: rat, Sprague-Dawley CD

Sex: male/female

Number of

Animals: 9

Vehicle: other: distilled water

Value: = 775 mg/kg bw

Method: other: Safepharm Standard Test Method Number 513.01

Year: 1998 **GLP:** yes

Test substance: other TS: Benzene sulfonic acid, C10-16-alkyl derivatives

(68584 - 22 - 5)

Method: A group of three fasted males was treated with the starting

dose (2000 mg/kg bw). As the females dosed with 2000 mg/kg bw died, a further three fasted males and three fasted females were treated with the dose level 300 mg/kg bw. The test material was administered orally as a solution in distilled water. The animals were observed 1/2, 1, 2, and 4 hours after dosing and then once daily for up to 14 days. Bodyweights were recorded on Day 0 (day of dosing) and on Days 7 and 14 or at death. At the end of the observation period the surviving animals were killed by cervical dislocation and all animals

were subject to gross necropsy.

Remark: LD50 value is geometric mean between 300 and 2000 mg/kg.

Three females were found dead one day after dosing at the 2000 mg/kg bw dose level. There were no deaths at the 300 mg/kg bw dose level. No clinical signs of toxicity were noted in animals treated with 300 mg/kg bw. The surviving animals showed expected gains in body weight over the study period. Abnormalities noted at necropsy of animals that died during the study were abnormally red lungs, dark liver, and dark

kidneys.

Source: Hempstock 1998.

Reliability: (1) valid without restriction

21-FEB-2003 (17)

Type: LD50

Species: other: rat, Wistar

Sex: male/female

Number of Animals:

Vehicle: no data

Value: = 500 - 2000 mg/kg bw

Method: OECD Guide-line 401 "Acute Oral Toxicity"

Year: 1987 GLP: yes

Test substance: other TS: Dodecylbenzenesulfonate, sodium salt as a surrogate

for benzene sulfonic acid, dodecyl- (27176-87-0)

Source: OECD 1987; IUCLID 1995.
Reliability: (2) valid with restrictions

Company reported GLP study listed in IUCLID Data Set but not

available for review.

02-JUL-2001 (20) (59)

Type: LD50 Species: rat

Sex: male/female

Number of

Animals: 10

Vehicle:

Value: = 1080 mg/kg bw

Method: OECD Guide-line 401 "Acute Oral Toxicity"
Year: 1981 GLP: no

Test substance: other TS: Marlon A 386 (CAS #68411-30-3) C10-13 LAS, average

alkyl chain length = C11.6; Activity: 86%

Method: Five male and five female rats were given LAS doses of 1075,

1220, 1360, 1710 or a control by gavage. Body weight and other signs were measured on days 7 and 14. Temperature was maintained at $20+/-1^{\circ}C$ with a 12 hr light-dark cycle. Animals

were observed for 14 days after dosing.

Remark: Symptoms beginning about 30 minutes past application included

diarrhea, squatting attitude, breathing difficulties, nose

bleeding, ataxia, and lethargy. These symptoms had

disappeared in surviving animals by 120 hours. Virtually all animals died in doses of 1220 mg/kg and above. Note that all doses are corrected for 86% activity. The original doses were

1250, 1415, 1580 and 1990 mg/kg.

Source: Murmann 1984a.

Reliability: (2) valid with restrictions

21-FEB-2003 (49)

- 33/55 -

Type: LD50

Species: other: Rat, CFY (Sprague-Dawley origin)

Sex: male/female

Number of

Animals: 10

Vehicle:

Value: = 1980 mg/kg bw

Method: OECD Guide-line 401 "Acute Oral Toxicity"

Year: GLP: yes

Test substance: other TS: Alkylbenzene sulfonate, sodium salt (designated as

P-500 N-Na).

Method: Five male and five female rats were given single doses by

gavage at 1500, 2350 and 3760 mg/kg bw. Rats were housed in cages grouped by sex and given standard laboratory diet and water ad libitum. Mean daily temperature was maintained at $21-22\,^{\circ}\mathrm{C}$ at a mean relative humidity of 56%. Lighting was on a

12 hrs dark and 12 hrs light photoperiod. Animals were

observed for 14 days after dosing.

Remark: Four rats from each of the two lowest concentrations and all

rats from the highest concentration died. All deaths occurred between 6 and 23 hours after dosing. Signs of reaction to treatment included pilo-erection, hunched posture, abnormal gait (waddling), lethargy, decreased respiratory rate, ptosis, pallor of the extremities, and diarrhea. All surviving animals appeared to recover completely by day 4. Autopsy of

animals appeared to recover completely by day 4. Autopsy of rats that died revealed isolated cases of pallor of the kidneys or spleen. Terminal necropsy findings for survivors were normal. Note that all doses are corrected for 47%

activity. The original doses were 3200, 5000, and 8000 mg/kg.

Source: Kynoch 1986a.

Test substance: Activity 47%. Average alkyl chain length = C11.2 Clear

yellow liquid.

Reliability: (1) valid without restriction

21-FEB-2003 (37)

5.1.2 Acute Inhalation Toxicity

Type: other: Approximate Lethal Concentration (ALC)

Species: other: Rat Crl: CD (SD) BR

Sex: male

Number of

Animals: 6

Vehicle:

Exposure time: 4 hour(s)

Value:

Method: other

Year: 1992 GLP: no data
Test substance: other TS: LAS (CAS #25155-30-0); activity 98%

Method: Groups of six male 8-week old rats were restrained in

perforated, stainless steel cylinders with conical nose

pieces. Exposure was nose-only to an aerosol atmosphere for 4 hours. After exposure, rats were returned to their cages and

observed for clinical signs for 14 days. Mean measured

- 34/55 -

concentrations in the test chambers were 65, 120, 260, and 310

mg/m3. Chamber temperature ranged between 25-26°C.

The ALC is defined as the lowest atmospheric concentration Remark:

generated that caused death in 1 or more rats either on the day of exposure or within 14 days post exposure. No mortality occurred at concentrations up to 260 mg/m3. At 310 mg/m3, one

rat died during exposure and 2 rats died one day post

exposure. The test material is considered moderately toxic by

inhalation. However, it is important to note that this

laboratory exposure is not representative of the possible LAS exposure during actual use. In this study, animals were given high exposures to respirable-sized particles. Spray products containing LAS are designed to produce large particle sizes. These large particles are needed for efficient delivery of the spray to the surface being cleaned. This results in particle sizes that are much larger than the respirable particle sizes used in testing and therefore would not be able to reach far into the lungs where effects could occur. Given this lack of relevance to real-world exposure potential, the use of this

study for risk assessment purposes is limited.

Result: 310 mg/m3 of particulate

Kinney 1985. Source:

Reliability: (2) valid with restrictions

21-FEB-2003 (29)

5.1.3 Acute Dermal Toxicity

LD50 Type: Species: rabbit

Sex:

Number of

Animals:

Vehicle:

= 2000 mg/kg bwValue:

Method: other: Test material was applied to shaved area of back of 6

rabbits at two doses: 2000 mg/kg (undiluted) and 212 mg/kg (2% aqueous dilution). The areas were covered with plastic and

left in contact with test material for 24 hours.

Year: GLP: no

Test substance: other TS: Benzene sulfonic acid, C10-16-alkyl derivatives

(68584 - 22 - 5)

All of the animals exposed to the 212 mg/kg survived. Remark:

Mortality occurred in three out of six rabbits exposed to the

undiluted dose. No untoward behavioral reactions were observed. Necropsy did not reveal any gross pathological alterations. Local skin reactions included erythema, mild edema and mild desquamation at 212 mg/kg and chemical burns,

severe edema and necrosis at 2000 mg/kg.

Result: LD50 = 2000 mg/kg bw (undiluted); LD50 > 212 mg/kg bw (2

aqueous dilution)

Source: Kretchmar 1972.

Reliability: (1) valid without restriction

21-FEB-2003 (31)

Type: LD50

Species: other: Rat, CFY (Sprague-Dawley origin)

Sex: male/female

Number of

Animals: 10

Vehicle:

Value: > 2000 mg/kg bw

Method: OECD Guide-line 402 "Acute dermal Toxicity"

Year: GLP: yes

Test substance: other TS: Alkylbenzene sulfonate, sodium salt (designated as

P-500 N-Na). activity 47%. Average alkyl chain length =

C11.2. Yellow, viscous liquid.

Method: Five male and five female rats were exposed to 2000 mg/kg in a

limit test. The test substance was applied to clipped intact skin in the dorso-lumbar region and covered with gauze held in place with an impermeable dressing. The dressing was removed after 24 hours and the treated area of the skin washed with

warm water and blotted dry. Observations for dermal

irritation were made daily for 14 days.

Remark: There were no deaths or signs of a systemic reaction following

a single dermal application at 2000 mg/kg bw. Well defined or slight erythema and slight oedema were observed at all test sites after removal of the occlusive dressing on Day 2. All test sites were entirely covered by scab formation from Day 7. Sloughing from the scabbed skin began at various times between Day 7 and Day 12 and was completed before termination. Low bodyweight gains or loss of body weight were recorded for one male and three females in Day 8. Two of the same females and a third female also showed low bodyweight gain between Days 8

and 15.

Source: Kynoch 1986b.

Reliability: (1) valid without restriction

21-FEB-2003 (38)

5.1.4 Acute Toxicity, other Routes

Type: Species: Sex:

Number of
Animals:
Vehicle:

Route of admin.:

Value: Method:

Year: GLP:

Test substance:

Remark: Not a required OECD or HPV endpoint.

08-FEB-2001

- 36/55 -

5.2 Corrosiveness and Irritation

5.2.1 Skin Irritation

Species: rabbit

Concentration: .5 other: mL

Exposure:

Exposure Time: 4 hour(s)

Number of

Animals: 6

PDII:

Result: highly irritating

EC classificat.: irritating

Method: OECD Guide-line 404 "Acute Dermal Irritation/Corrosion"

Year: 1981 **GLP:** yes

Test substance: other TS: Benzenesulfonic acid, C10-13-alkyl derivatives

(85536-14-7) as a surrogate for benzene sulfonic acid,

C10-16-alkyl derivatives (68584-22-5)

Remark: The shaved treated area was covered for the first 4 hours.

Observations were made after 1, 24, 48, 72 hours and 6, 9, and

14 days. The irritation index was 5.25.

Source: Murman 1984; OECD 1981.

Reliability: (1) valid without restriction

20-FEB-2003 (48) (53)

Species: rabbit

Concentration: .5 other: mL

Exposure:

Exposure Time: 4 hour(s)

Number of

Animals: 6

PDII:

Result: corrosive
EC classificat.: irritating
Method: Draize Test

Year: 1965 GLP:

Test substance: other TS: Benzene sulfonic acid dodecyl- (27176-87-0)

Method: The test material was applied as submitted to the intact skin

and covered with a "1 x 1" gauze patch held in place with saran wrap. At the end of 4 hours, the coverings were removed

and the area examined for skin irritation and corrosion. Examinations were repeated at 24 and 48 hours and scored

according to Draize 1965.

Remark: The primary dermal irritation scores were 3.4, 6.3, and 7.0 at

4, 24, and 48 hours, respectively.

Source: Thompson 1980.

Reliability: (1) valid without restriction

02-NOV-2001 (1) (11) (71)

Species: other: New Zealand albino rabbits

Concentration: .5 other: mL

Exposure:

Exposure Time: 4 hour(s)

Number of Animals:

PDII:

Result: moderately irritating

EC classificat.:

Method: OECD Guide-line 404 "Acute Dermal Irritation/Corrosion"

Year: GLP: yes

Test substance: other TS: Alkylbenzene sulfonate, sodium salt (designated as

P-500 N-Na). Activity 47%. Average alkyl chain length =

C11.2. Clear yellow liquid.

Method: A 0.5 ml aliquot of P-500 N-Na was applied under a 2.5 cm2

gauze pad to an approximate 10 cm2 area of clipped intact skin of 3 rabbits. Each treatment site was occluded with an elastic adhesive dressing for four hours, after which the dressing was removed and the area washed with distilled water. Examination of the treated skin was made approximately 30 minutes after removal of the patch and daily through 14 days.

Grading and scoring of the dermal reactions was performed

using the standard numerical scoring system.

Remark: Well defined to moderate skin reactions were observed in all

three animals following removal of the bandages. Desquamation of the stratum corneum was observed in all three animals. The reaction in all three animals gradually ameliorated from Days 5, 10 and 11, respectively, and had all resolved completely in

one animal by Day 12.

Source: Liggett and Parcell 1986a.
Reliability: (1) valid without restriction

21-FEB-2003 (41)

5.2.2 Eye Irritation

Species: rabbit

Concentration: .1 other: mL

Dose:

Exposure Time: 144 hour(s)

Comment: Number of

Animals: 6

Result: moderately irritating

EC classificat.: irritating

Method: OECD Guide-line 405 "Acute Eye Irritation/Corrosion"

Year: 1981 GLP: no

Test substance: other TS: Benzenesulfonic acid, C10-13-alkyl derivatives

(85536-14-7) as a surrogate for benzene sulfonic acid,

C10-16-alkyl derivatives (68584-22-5)

Remark: Treatment was to the right eye with lower lid removed. The

left eye was untreated. The eyes were not washed out during the test. Observations were made at 1, 24, 48, and 72 hours

- 38/55 -

and at 6 days after application. The total irritation index

was 46.9.

Source: Murmann 1984; OECD 1981.

Reliability: (1) valid without restriction

20-FEB-2003 (47) (54)

Species: other: New Zealand albino rabbits

Concentration: .1 other: mL

Dose:

Exposure Time:

Comment: Number of

Animals:

Result: irritating

EC classificat.:

Method: OECD Guide-line 405 "Acute Eye Irritation/Corrosion"

Year: 1981 GLP: yes

Test substance: other TS: Alkylbenzene sulfonate, sodium salt (designated as

P-500 N-Na). Activity 47%. Average alkyl chain length =

C11.2. Clear yellow liquid.

Method: Nine rabbits received a 0.1 mL aliquot of P-500 N-Na placed

into the lower everted lid of one eye per animal. For three rabbits the eyelids were then gently held together for one second before releasing. For three other rabbits the eyes were irrigated with water for 5 minutes following a 4-second exposure. For the remaining three rabbits the eyes were irrigated for 5 minutes following a 30-second exposure. Eyes were examined after 1 hour and 1, 2, 3, 4, 7, 14 and 21 days after exposure. Grading was performed using the standard

scoring system.

Remark: The following results were noted:

1) Three animals without any rinsing: averaged irritation scores (24, 48, 72 hours) for each animal: cornea 2.3, 1.7, 2; iris: 1.3, 0, 0; conjunctivae redness: 3, 1.7, 2; conjunctivae chemosis: 3, 2, 2. In the first animal the effects were persistent at day 14.

2) Three animals with rinsing for five minutes following a 30 second exposure: averaged scores: cornea 0.7, 1, 1.3; iris: 0, 0.7, 0.3; conjunctivae redness: 1.7, 2, 1.3; conjunctivae chemosis: 2, 1.3, 2. The eyes were normal 7 or 14 days after instillation.

3) Three animals with rinsing for five minutes following a 4 second exposure: averaged scores: cornea 0.7, 2.3, 0.7; iris: 0, 0, 0; conjunctivae redness: 1.7, 1.7, 1; conjunctivae chemosis: 1.3, 2, 1. The eyes were normal 7 days after instillation.

Findings lead to a definition of irritating for LAS at 47% applied without rinsing, irritating (even if with lower effects, mainly as cornea opacity and conjunctivae redness) with rinsing after 30 second of exposure, and not irritating

- 39/55 -

with rinsing after 4 second of exposure.

Overall, instillation of P-500 N-Na into the eyes of rabbits elicited positive responses in all animals. Irrigation of the

eyes only slightly reduced the irritation potential.

Source: Liggett and Parcell 1986b.
Reliability: (1) valid without restriction

21-FEB-2003 (42)

5.3 Sensitization

Type: other: sensitization

Species: guinea pig

Number of

Animals: 20

Vehicle: other: corn oil **Result:** not sensitizing

Classification:

Method: other: Magnusson and Kligman

Year: 1969 **GLP:** yes

Test substance: other TS: Dobanic acid 103 (Benzenesulfonic acid, C10-13) as a

surrogate for benzene sulfonic acid, C10-16-alkyl derivatives

(68584 - 22 - 5)

Remark: In a guinea-pig maximization test none of the test animals

showed positive responses at 24 or 48 hours after removal of

the challenge patches. The test material showed no

sensitizing potential in guinea pigs.

Source: Rose 1983.

Reliability: (1) valid without restriction

21-JAN-2002 (44) (66)

Type: Guinea pig maximization test Species: other: guinea pig, Hartley

Number of

Animals: 20
Vehicle: water

Result: not sensitizing Classification: not sensitizing

Method: other: OECD Guideline 406; Directive 179/831 Annex, Part B.

Year: 1981 GLP: yes

Test substance: other TS: LAS, activity: 50%; average alkyl chain length =

C11.6

Remark: Solutions of LAS were applied intracutaneously and

epicutaneously to 10 male and 10 female animals. Induction concentration was 25% in water; the challenge concentration

was 12.5%. No positive responses were observed.

Source: RBM 1985.

Reliability: (1) valid without restriction

21-FEB-2003 (64)

5.4 Repeated Dose Toxicity

Species: rat Sex: male/female

Strain: Wistar

Route of admin.: drinking water

Exposure period: 9 months

Frequency of

treatment: Daily in drinking water

Post. obs. period:

Doses: 0.07, 0.2%, 0.6% (85, 145, 430 mg/kg bw d)

Control Group: yes

NOAEL: = 85 mg/kg bw

LOAEL: = 145

Method: other: Groups of 8-9 male and 8-9 female rats were given LAS

for 9 months.

Year: GLP: no

Test substance: other TS: C10-14 LAS (CAS #69669-44-9); average alkyl chain

length (based on LAS SIDS Consortium Survey, 2000) = C11.7

Remark: Information as cited in IPCS document. This study represents

the most appropriate NOAEL value identified by the Industry Coalition for the SIDS Assessment of LAS (LAS Coalition). The LAS Coalition reviewed fifteen studies in which rodents (rats

and mice) and non-rodents (monkeys) received repeated exposures to LAS via the oral or dermal routes. Test

durations ranged from 15 days up to 9 months in those studies. LOAELs ranged from 115 to 750 mg/kg bwd and the highest NOAEL (below the lowest LOAEL) was found to be the 85 mg/kg bwd

resulting from the study summarized here.

Result: Body weight gain was suppressed in the male 0.6% group.

Haematological, serum-biochemical, and enzymatic parameters of

the liver and kidney were also affected in the high dose groups. No organ weight changes were observed. The intake of LAS was 50~mg/kg bw d in the male 0.07% group. The values for

the 0.2% group were 120 and 170 mg/kg bw d for males and

females, respectively.

Source: European Commission 2000a; Yoneyama et al. 1976.

Reliability: (4) not assignable

21-MAR-2003 (12) (81)

- 41/55 -

5.5 Genetic Toxicity 'in Vitro'

Type: other: Bacterial reverse mutation assay (Ames test)

System of

testing: Salmonella typhimurium TA 98 and TA 100

Concentration: 1.5 to 1500 ug/plate

Metabolic

activation: with and without

Result: negative Method: other: Ames

Year: GLP: yes

Test substance: other TS: Benzene sulfonic acid, C10-16-alkyl derivatives

(68584 - 22 - 5)

Remark: The test material was tested up to its toxic limit.

Result: No significant increases in the frequency of revertant colonies were recorded for either of the bacterial strains

with any dose of the test substance, either with or without

metabolic activation.

Source: Thompson 1998.

Reliability: (1) valid without restriction

05-NOV-2001 (72)

Type: Ames test

System of

testing: Salmonella typhimurium TA 1535, TA 1537, TA 1538, TA 98, TA

100

Concentration: 8-5000 ug/plate

Metabolic

activation: with and without

Result: negative

Method: Directive 84/449/EEC, B.14 "Other effects - Mutagenicity

(Salmonella typhimurium - reverse mutation assay)"

Year: 1984 GLP: yes

Test substance: other TS: Marlon A 390 (CAS #68411-30-3) C10-13 LAS, average

alkyl chain length = C11.6; activity 91.3%

Remark: Negative and positive controls used.

Result: Cytotoxicity concentration:

With metabolic activation: > 5000 ug/plate Without metabolic activation: > 5000 ug/plate

Source: EEC Directive 1984; Schoeberl 1993a.

Reliability: (1) valid without restriction

21-FEB-2003 (8) (68)

- 42/55 -

Type: other: transformation test with SHE-cells

System of

testing: Syrian hamster embryo (SHE) cells

Concentration: up to 50 ug/ml

Metabolic

activation: without
Result: negative

Method:

Year: GLP: no

Test substance: other TS: C10-14 LAS, sodium salts (CAS #69669-44-9)

Method: Cell cultures were prepared and plated in 75 cm2 flasks

Method: Cell cultures were prepared and plated in 75 cm2 flasks containing 20 mL of culture medium. On day 5, target cells

were trypsinized and a suspension of target cells was added to the solution plated on complete medium. Plates were dosed on day 6. Nine dishes were used for each dose level. On day 14, the cultures were fixed, stained, and examined to count normal

and transformed colonies.

Remark: LAS did not produce transformation at any of the doses tested.

Source: Inoue et al. 1980.

Test substance: average alkyl chain length (based on LAS SIDS Consortium

Survey, 2000) = C11.7; activity: 22.2%

Reliability: (2) valid with restrictions

21-FEB-2003 (26)

5.6 Genetic Toxicity 'in Vivo'

Type: Micronucleus assay

Species: mouse Sex: male/female

Strain: NMRI

Route of admin.: other: oral intubation

Exposure period: 72 hours

Doses: 1122 mg/kg

Result: negative

Method: OECD Guide-line 474 "Genetic Toxicology: Micronucleus Test"

Year: 1983 **GLP:** yes

Test substance: other TS: Benzenesulfonic acid, C10-13-alkyl derivatives

(85536-14-7) as a surrogate for benzene sulfonic acid,

C10-16-alkyl derivatives (68584-22-5)

Remark: No significant increases in the number of polychromatic

erythrocytes with micronuclei were observed.

Source: Fedtke 1991; OECD 1983.

Reliability: (1) valid without restriction

11-OCT-2001 (13) (55)

- 43/55 -

other: Mammalian bone marrow cytogenetic assay Type: other: mouse: ICR: JCL Species:

Strain: TCR

Route of admin.: gavage
Exposure period: 5 days and 1 day Doses: 200, 400, 800 mg/kg

Result: negative

Control Group: other: yes, concurrent no treatment, positive, and historical

controls

Method: other: Chromosomal aberrations were examined 6, 24, 48 hours

> after administration. Mytomycin C was used as a positive control at a dose of 5 mg/kg and induced severe chromosomal aberrations.

Year: GLP: no

Test substance: other TS: C10-14 LAS, sodium salt (CAS #69669-44-9); average

alkyl chain length (based on LAS SIDS Consortium Survey, 2000)

Besides the pure LAS, commercial preparation containing 19% Remark:

LAS and another containing 17.1% LAS were given to mice as single doses only by gavage at 800, 1600 or 3200 mg/kg bw d and 1000, 2000 or 4000 mg/kg bw d, respectively. The highest doses were 50% of the respective LD50 values. No significant differences in the incidence of chromosomal aberrations were

observed in any LAS treatment relative to the controls.

Information as cited in the IPCS document.

Result: There was no significant difference in the incidence of

chromosomal aberrations between any of the groups given LAS

and the negative control group.

Inoue et al. 1977; European Commission 2000a. Source:

Reliability: (4) not assignable

20-FEB-2003 (12) (25)

5.7 Carcinogenicity

Species: Sex: male/female

Strain: other: Charles River

Route of admin.: oral feed Exposure period: 2 years

Frequency of

treatment: continuous in feed

Post. obs. period:

0.02, 0.1, 0.5% (10, 50, 250 mg/kg bw d Doses:

Result:

Control Group: other: yes, concurrent no treatment and historical controls

Method:

GLP: no

other TS: C10-14 LAS, sodium salt (CAS# 69669-44-9); 98.1% Test substance:

activity on an anhydrous basis (41.9% active)

Method: Four groups of Charles River weanling rats, divided by sex,

were given 0.5, 0.1, and 0.02% LAS in their food for 2 years. Following completion of those studies, five male and five female rats from each of the parental groups (F1b and F2b) and all survivors were selected for necropsy. Body weight and organ to body weight ratios were recorded, and routine

hematology and histology were performed. Weanling animals for

- 44/55 -

the F3a generation were similarly treated.

Result: Gross examination of all animals for pathology did not reveal

any abnormalities. No consistent dietary induced changes that could be considered a toxic response were observed. Animals that showed significant loss of weight, development of tumors, or other evidence of abnormalities were sacrificed and tissues examined. The incidence of tumors and the common incidental

diseases were similar in all dieting groups.

Source: Buehler et al. 1971.

Reliability: (2) valid with restrictions

27-MAR-2003 (2)

5.8 Toxicity to Reproduction

Type: other: 3-generation reproduction study

Species: rat Sex: male/female

Strain: other: Charles River

Route of admin.: oral feed
Exposure Period: 2 years

Frequency of

treatment: continuous in feed

Premating Exposure Period
male: 84 days
female: 84 days

Duration of test: 3 generations

Doses: 0.02, 0.1, 0.5% (14, 70, 350 mg/kg bw d)

Control Group: yes

NOAEL Parental: = 350 mg/kg bw NOAEL F1 Offspr.: = 350 mg/kg bw NOAEL F2 Offspr.: = 350 mg/kg bw

Method:

Year: 1971 **GLP:** no

Test substance: other TS: Sodium salt LAS (C10-14), activity: 98.1% on an

anhydrous basis (41.9% active)

Method: Na-LAS (chain length distribution C10-14) was fed for 84 days

to 4 groups of weanling rats (3 dose levels, plus control),

each dose consisting of 50 animals each of both sexes

(PO-generation). When the PO generation was 107-112 days old, 20 females from each dose group were mated with 20 males from the same group and maintained together for 17 days. The first litters of each generation (Fla- and F2a-generation) were sacrificed at 21 days of age. Ten days after the final litter was sacrificed, all females were remated with different males from the same group to obtain the F1b generation. From the F1b-generation, 20 males and females of each group were

be used for further reproduction studies. Reproduction studies on the F1b and F2b generations were started when the rats were 80 to 85 days old, and were continued until the F3b

selected at weaning to continue their respective diets and to

generation was weaned.

Result: Results were reported as no effects at the highest

concentration tested (0.5% in the diet). General reproduction

including fertility gestation, parturition, neonatal

viability, lactation, and post-weaning growth was normal for all test groups and did not deviate from the controls in each generation. No gross abnormalities were noted. No definitive adverse effects due to the test material were noted in the

haematology and pathology.

Source: Buehler et al. 1971.

Reliability: (2) valid with restrictions

20-FEB-2003 (2)

5.9 Developmental Toxicity/Teratogenicity

Species: rat Sex: female

Strain: other: SD-JCL
Route of admin.: oral feed

Exposure period: from day 0 to 20 of gestation

Frequency of

treatment: daily

Duration of test:

Doses: 0.1%, 1.0% (80, 780 mg/kg bw d)

Control Group: yes

NOAEL Maternalt.: = 780 mg/kg bw NOAEL Teratogen.: = 780 mg/kg bw

Method: other: LAS was fed in the diet to 16 pregnant female rats/dose

from day 0 to 20 of gestation.

Year: GLP: no

Test substance: other TS: Japan LAS; average alkyl chain length (based on LAS

SIDS Consortium Survey, 2002) = C11.7-12.3.

Remark: Information as cited in IUCLID Data Sheet and IPCS document.

This study represents the most appropriate NOAEL value

identified by the Industry Coalition for the SIDS Assessment of LAS. The LAS Coalition reviewed ten developmental toxicity studies conducted on rats, mice and rabbits in which the test animals received LAS via the oral route (feed, gavage, or drinking water). While effects were observed at maternally toxic doses, no decreases in litter size, no changes in litter parameters, and no malformations or significant differences in skeletal defects were observed in these studies at oral doses

up to 780 mg/kg bwd. Note also that the NOAEL used in the risk assessment is derived from the repeated dose studies.

Result: The LAS intake was about 780 mg/kg with the 1% diet, but there

were no abnormalities in the body weight gains of the dams, or in the occurrence and maintenance of pregnancy. The values of

the litter parameters did not differ from those of the controls and there was no evidence of teratogenicity. The numbers of offspring were rather low in the 1% group, and the weaning rate of 78.3% was lower than the 100% rate observed in the controls. However, there were no abnormalities in body weight gain, organ weights or functions in the offspring.

Source: European Commission 2000a; Tiba et al. 1976.

Reliability: (4) not assignable

21-MAR-2003 (12) (73)

Species: mouse Sex: female

Strain: ICR
Route of admin.: dermal

Exposure period: from day 6 through day 15 of pregnancy

Frequency of

treatment: daily

Duration of test:

Doses: 0.03, 0.3, 3% (15, 150, and 1500 mg/kg bw d)

Control Group: yes
NOAEL Maternalt.: = 150 mg/kg bw

NOAEL Teratogen: = 1500 mg/kg bw

Method: other: Areas of 4 x 4 cm on the backs of the mice were

depilated and aqueous solutions of LAS were applied.

Year: GLP: no

Test substance: other TS: C10-14 LAS (CAS #69669-44-9); average alkyl chain

length (based on LAS SIDS Consortium Survey, 2002) = C11.7;

activity: 46.6%

Remark: Information as cited in the IUCLID Data Sheet and the IPCS

document. This study represents the most appropriate NOAEL value identified by the Industry Coalition for the SIDS Assessment of LAS. The LAS Coalition reviewed seven

developmental toxicity studies conducted on rats, mice and rabbits in which the test animals received LAS via the dermal route. While effects were observed at maternally toxic doses, no decreases in litter size, no changes in litter parameters, and no malformations or significant differences in skeletal defects were observed in these studies at dermal doses up to 1,500 mg/kg bwd. Note also that the NOAEL used in the risk

assessment is derived from the repeated dose studies.

Result: The 3% group showed a clear decrease in the pregnancy rate

(67.9%) when compared with a rate of 96.3% in the controls. However, there were no decreases in the litter size, and no changes in the litter parameters with the exception of a slight decrease in fetal body weight. There were no

significant increases in the incidence of malformations in the

fetuses.

Source: European Commission 2000a; Imahori et al. 1976.

Reliability: (4) not assignable

21-MAR-2003 (12) (24)

5.10 Other Relevant Information

Type:

Remark: None

11-OCT-2001

5.11 Experience with Human Exposure

Memo: LAS has been extensively studied and used for many years

without significant incidents.

11-OCT-2001

- 47/55 -

(1) 49 CFR 173.1200 Appendix A. Method of testing corrosion to the skin.

- (2) Buehler, E.V., Newmann, E.A., and King, W.R. 1971. Two year feeding and reproduction study in rats with linear alkylbenzene sulfonate (LAS). Toxicol. Appl. Pharmacol. 18:83-91.
- (3) Cohen, L., Vergara, R., Moreno, A. and Berna, J.L. 1995. Influence of 2-phenyl alkane and telralin content on solubility and viscosity of linear alkylbenzene sulfonate. JAOCS 72:115-122.
- (4) CONDEA Vista. 1995. Material Safety Data Sheet for VISTA SA-597L Sulfonic Acid, Revision No. 02/95, last revised 4/24/95.
- (5) Cross, J. and Dekker, M. (ed.). 1977. Anionic surfactants: Chemical analysis, v. 8, p. 111-115.
- (6) Deutsche Einheitsverfahren zur Wasser-, Abwasser- und Schlamm-untersuchung. L 11: Bestimmung der Wirkung von Wasserinhaltsstoffen auf Kleinkrebse (Daphnien-Kurzzeittest). DIN 38412 Teil 11.
- (7) Deutsche Einheitsverfahren zur Wasser-, Abwasser-, und Schlammuntersuchung. L 15: Bestimmung der Wirkung von Wasserinhaltsstoffen auf Fische - Fischtest DIN 38412 Teil 15.
- (8) Directive 84/449/EEC, B.14 mutagenicity. 1984. Salmonella typhimurium-reverse mutation assay.
- (9) Directive 84/449/EEC, C.2. 1984. Acute toxicity for Daphnia.
- (10) Douglas, M.T., Chanter, D.O., Pell, I.B., and Burney, G.M. 1986. A proposal for the reduction of animal numbers required for the acute toxicity to fish test (LC50 determination). Aquat. Toxicol. 8:243-249.
- (11) Draize, J.H. 1965. Appraisal of the safety of chemicals in foods, drugs, and cosmetics-dermal toxicity. Association of Food and Drug Officials of the U.S., Topeka, Kansas Pp. 46-59.
- (12) European Commission. 2000a. Benzenesulfonic acid, C10-13-alkyl derivs., sodium salts. Year 2000 CD-ROM edition.

- 48/55 -

(13) Fedtke, N. 1991. Mutagenitatsprufung von Marlon AS 3 im in vivo mikrokerntest an der maus. Report No. MK-91/0026.

- (14) Freitag, D., Ballhorn, L., Geyer, H., and Korte, F. 1985. An experimental method for the assessment of the behaviour of organic chemicals in the ecosphere by means of simple laboratory tests with C14 labelled chemicals. Chemosphere 14:1589-1616.
- (15) Galassi et al. 1992. Water Res. 26:19-27 as cited in IUCLID. 1995. IUCLUD data sheet: dodecylbenzenesulfonic acid.
- (16) Hand, V.C. and Williams, G.K. 1987. Structure-activity relationships for sorption of linear alkylbenzenesulfonates. Environ. Sci. Technol. 21:370-373.
- (17) Hempstock, C. 1998. NEOPELEX FS: Acute oral toxicity study in the rat - Acute toxic class method. SPL Project No. 140/854.
- (18) HERA. 2002. HERA-LAS Human and Environmental Risk Assessment: Linear Alkylbenzene Sulphonates, LAS. CAS No. 68411-30-3, Draft #6, May 2002.
- (19) Hoechst AG. 1988. Unveroffentlichte unters. ber. 88.0913. as cited in IUCLID. 1995. IUCLID data sheet: dodecylbenzenesulfonic acid.
- (20) Hoechst AG. 1988. Unveroffentlichte unters. ber. 88.0925. as cited in IUCLID. 1995. IUCLID data sheet: dodecylbenzenesulfonic acid.
- (21) Huels. 1993. Huels report No. DDA-21.
- (22) Huntsman 2002. Report on the melting point analysis for NANSA HS 85/S. Attached technical bulletin dated 04-01-1994. Cover memo from A. Ashworth to K.B. Sellstrom dated April 12, 2002.
- (23) Huntsman. 2002. Report of melting point analysis for NANSA HS 85/5. Cover memo from A. Ashworth to K.B. Sellstrom dated April 12, 2002.
- (24) Imahori, A., Kinagawa, T. and Shiobara, S. 1976. Effects of linear alkyl benzene sulfonate (LAS) applied dermally to pregnant mice and their fetuses. Jpn. J. Public Health. 23:68-72 (in Japanese); cited in IPCS (1996); Environmental Health Criteria 169: Linear Aklylbenzene Sulfonates (LAS) and Related Compounds. WHO, Geneva, Switzerland.

- 49/55 -

(25) Inoue, K., Shibata, T., Hamano, Y., Oda, Y., Kuwano, A., Yamamoto, H., Mitsuda, B. and Kunita, N. 1977. In vivo cytogenetic tests of some synthetic detergents in mice. Ann Res. Osaka Prefect Inst. Public Health. 8:17-24 (in Japanese); cited in: IPCS (1996); Environmental Health Criteria 169: Linear Aklylbenzene Sulfonates (LAS) and Related Compounds. WHO, Geneva, Switzerland.

- (26) Inoue, K., Sunakawa, T., and Takayama. 1980. Studies of in vitro cell transformation and mutagenicity by surfactants and other compounds. Fd. Cosmet. Toxicol. 18:289-296.
- (27) IUCLID. 1995. IUCLID data sheet: Benzenesulfonic acid, C10-16-alkyl derivatives.
- (28) IUCLID. 1995. IUCLID data sheet: Dodecylbenzenesulphonic acid.
- (29) Kinney, L.A. 1985. Approximate lethal concentrations (ALCs) by inhalation of sodium lauryl sulfate & sodium dodecylbenzene sulfonate. Dupont Haskell Laboratory Report No. 474-84.
- (30) Knie, V.J., Halke, A., Juhnke, I., and Schiller, W. 1983. Ergebnisse der untersuchungen von chemischen stoffen mit vier biotests (Results of studies on chemical substances with four biotests). Deutsch Gewasserkundliche Mitteilungen 77-79.
- (31) Kretchmar. 1972. Acute toxicity studies with XTW-1226. Report to Procter & Gamble Company, IBT No. A1717.
- (32) Kurtin. 1994. Bestimmung der Auswirkungen von Marlon AS 3 auf das wachstum von Scendesmus subscipicatus 86.81.SAG. Report No. AW-371.
- (33) Kurtin. 1994. Bestimmung der biologischen Abbaubarkeit von Marlon AS 3 im DOC-Die-Away test. Report No. DDA-79.
- (34) Kurtin. 1994. Bestimmung der biologischen Abbaubarkeit von Marlon AS 3 im modifizierten coupled units-test. Report No. MCU-21.
- (35) Kurtin. 1995. Bestimmung der auswirkungen von MARLON AS 3 auf das schwimmverhalten von Daphnic magna. Report No. DK-620.
- (36) Kurtin. 1997. Bestimmung der akuten wirkungen von MARLON AS 3 gegenuber fischen. Report No. FK-1375.

- 50/55 -

(37) Kynoch, S.R. 1986a. Acute oral toxicity to rats: P-500 N-Na. Huntingdon Research Cener Report. No. 86546D/PEQ 7/AC.

- (38) Kynoch, S.R. 1986b. Acute dermal toxicity to rats of P-500 N-Na. Huntingdon Research Center. Report No. 86718D/PEQ 8/AC.
- (39) Leo, A.J. and Hansch, C. 1979. Substituent Constants for Correlation Analysis in Chemistry and Biology. J. Wiley & Sons, N.Y.
- (40) Lide, D.R. 1990. Handbook of Chemistry and Physics. 71st Edition. CRC Press: Ann Arbor.
- (41) Liggett, M.P. and Parcell, B.I. 1986a. Irritant effects on rabbit skin of P-500 N-Na. Huntingdon Research Center. Report No. 86400D/PEQ 9/SE.
- (42) Liggett, M.P. and Parcell, B.I. 1986b. Irritant effects on the rabbit eye of P-500 N-Na. Huntingdon Research Center Report No. 86570D/PEQ 10/SE.
- (43) Lyman, W.J. 1985. Environmental exposure from chemicals, V.I, p.31, Neely, W.B., and Blau, G.E., editors. CRC Press. Boca Raton.
- (44) Magnusson, B. and Kligman, A.M. 1969. The identification of contact allergens by animal assay: The guinea pig maximization test. J. Invest. Dermatol. 52:268-276.
- (45) Matsuura, T. and Smith, J.M. 1970. Kinetics of photodecomposition of dodecyl benzene sulfonate. Ing. Eng. Chem. Fund. 9:252-260.
- (46) Murmann, P. 1984. Acute orale toxizitat von Marlon AS 3-Saure fur ratten. Report No. 0303.
- (47) Murmann, P. 1984. Prufung der akuten augen- und schleimhautreizwirkung von Marlon AS 3-saure. Report No. 0305.
- (48) Murmann, P. 1984. Prufung der akuten hautreizwirkung von Marlon AS 3-Saure. Report No. 0304.
- (49) Murmann, P. 1984a. Akute orale Toxizitat von Marlon A 386 fur Ratten. Huels Report No. 0191.
- (50) Noeller, C.R. 1966. Textbook of Organic Chemistry. 3rd Edition. W.B. Saunders Company: Philadelphia.

- 51/55 -

(51) Organisation for Economic Co-operation and Development (OECD). 1981. OECD guidelines for the testing of chemicals 305E.

- (52) Organisation for Economic Co-operation and Development (OECD). 1981. OECD guidelines for the testing of chemicals No. 401.
- (53) Organisation for Economic Co-operation and Development (OECD). 1981. OECD guidelines for the testing of chemicals No. 404.
- (54) Organisation for Economic Co-operation and Development (OECD). 1981. OECD guidelines for the testing of chemicals No. 405.
- (55) Organisation for Economic Co-operation and Development (OECD). 1983. OECD guidelines for the testing of chemicals No. 474.
- (56) Organisation for Economic Co-operation and Development (OECD). 1984. OECD guidelines for the testing of chemicals No. 201.
- (57) Organisation for Economic Co-operation and Development (OECD). 1984. OECD guidelines for the testing of chemicals No. 202.
- (58) Organisation for Economic Co-operation and Development (OECD). 1984. OECD guidelines for the testing of chemicals, No. 203.
- (59) Organisation for Economic Co-operation and Development (OECD). 1987. OECD guidelines for the testing of chemicals, No. 401.
- (60) Organisation for Economic Co-operation and Development (OECD). 1992. OECD guidelines for the testing of chemicals, No. 203.
- (61) Organisation for Economic Co-operation and Development (OECD). 1992. OECD guidelines for the testing of chemicals, No. 301B.
- (62) Organisation for Economic Co-operation and Development (OECD). 1995. OECD guidelines for the testing of chemicals, No. 202.
- (63) Procter & Gamble. 1991. AT/17.

- 52/55 -

(64) RBM. 1985. Test di sensibilizzazione cutanea nella cavia. RBM Exp. No. 2076.

- (65) Roberts, D.W. 1991. QSAR issues in aquatic toxicity of surfactants. Sci. Total Environ. 109/110:557-568.
- (66) Rose, G.P. 1983. Toxicology of detergents: The skin sensitizing potential of Dobanic acid 103. Group research report SBGR.83.383.
- (67) Schoberl, P. 1991. Coupling the OECD confirmatory-test with continuous ecotoxicity tests. Communication 1: Modification of the OECD confirmatory test (sewage treatment plant simulation model). Tenside Surfactants Detergents 6.
- (68) Schoeberl, P. 1993a. Bestimmung der Mutagenitat von Marlon A 390 im Salmonella/Sauger-Mikrosomen-Mutagenitatstest nach Ames. Huels Final Report No. AM-93/12.
- (69) Stepan Company. Biotic degradation (modified Sturm test) evaluation, in an aqueous medium, of the "ultimate" biodegradability of substances: 1736-1A, 1736-1B, 1736-1C, 1736-1D, 1736-1E. Ineris-Study 16 BF 53.
- (70) Stephenson, R.R. 1981. Dobanic acid 102: Acute toxicity to Salmo gairdneri, Daphnia magna, and Selenstrum capricornutum. Group research preport SBGR.81.083.
- (71) Thompson, G.W. 1980. D.O.T. skin corrosivity-method, summary for Bio-Soft S-100. Raltech Scientific Services. Lab Study No. 793159.
- (72) Thompson, P.W. 1998. NEOPELEX FS: Reverse mutation assay "Ames test" using Salmonella typhimurium strains TA 98 and TA 100 single experiment. SLP Project No. 140/855.
- (73) Tiba, S., Shiobara, S., Imahori, A. and Kitagawa, T. 1976. Effects of linear alkylbenzene sulfonate on dam, fetus and newborn rat. J. Food Hyg. Soc. Jpn. 17:66-71. (In Japanese); cited in IPCS. 1996. Environmental Health Criteria 169: Linear Alkylbenzene Sulfonates and Related Compounds. World Health Organization, Geneva, Switzerland. Original article in Japanese.
- (74) Tolls, J., Haller, M., DeGraaf, I., Thijssenk, M.A.T.C., and Sijm, D.T.H.M. 1997. Bioconcentration of LAS: Experimental determination and extrapolation to environmental mixtures. Environ. Sci. Technol. 31:3426-3431.

- 53/55 -

- (75) USEPA 1985.
- (76) USEPA. 2000. EpiSuite Estimation Software V.3.10. US Environmental Protection Agency.
- (77) van de Plassche, E.J., DeBruijn, J.H.M., Stephenson, R.R., Marshall, S.J., Feijtel, T.C.J., and Belanger, S.E. 1999. Predicted no-effect concentrations and risk characterization of four surfactants: Linear alkyl benzene sulfonate, alcohol ethoxylates, alcohol ethoxylated sulfates, and soap. Environ. Toxicol. Chem. 18: 2653-2663.
- (78) Verge, C. and Moreno, A. 1996. Toxicity of anionic surfactants to green microalgae "Scenedesmus subspicatus" and "Selenastrum capricornutum". Tenside Surf. Det. 33:166-168.
- (79) Verge, C. and Moreno, A. 2000. Effects of anionic surfactant on Daphnia magna. Tenside Surf. Det. 37:172-175.
- (80) Verschueren, K. 1996. Handbook of Environmental Data on Organic Chemicals, Third Edition. New York: John Wiley & Sons, Inc.
- (81) Yoneyama, M., Mabuchi, Y., Ikawa, M., Kobayashi, H. and Ichikawa, H. 1976. Subacute toxicity of linear alkylbenzene sulfonate. Ann. Rep. Tokyo Metr. Res. Lab. Public Health 27:105-112 (in Japanese); cited in: IPCS (1996); Environmental Heath Criteria 169: Linear Aklylbenzene Sulfonates (LAS) and Related Compounds. WHO Geneva, Switzerland.

- 54/55 -

date: 27-MAR-2003

7. Risk Assessment Substance ID: LABSA

7.1 Risk Assessment

Memo: See LAB sulfonic acids assessment plan.

21-MAR-2003

- 55/55 -